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Table of contents

Molecular Scope: watching macromolecular dynamics at solid-liquid interfaces at the single-chain level

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Molecular-scale interactions between polymers in solution and solid surfaces govern a large number of macroscopic processes in soft matter, from surface functionalization to hydrogel friction. Despite extensive characterization of these processes at the macroscopic level, our molecular understanding of polymer/surface interactions remains scarce, particularly under out-of-equilibrium situations. Here, we couple state-of-the-art single-molecule microscopy techniques with microfluidic transport, to directly track the nanoscale dynamics of single fluorescently tagged PEG macromolecules at solid/liquid interfaces, allowing to probe their subtle couplings with interfacial hydrodynamic flows.

In the absence of hydrodynamic forces, we uncover an heterogeneous and strongly non-Brownian surface diffusion for individual chains, which alternate between a low-mobility adsorbed state and long desorption-mediated jumps through the solvent (1, 2). The symmetry-breaking effect of the flow leads to a skewed distribution of interfacial displacements, with an unexpected dependence on the nature of the surfaces. On sticky hydrophilic surfaces, the hydrodynamic flow does not affect the chain motion except for an advective effect during solvent-mediated flights. On slippery hydrophobic surfaces, we instead evidence a peculiar regime of mixed macromolecular friction, whereby the adsorbed chain rubs on the solid wall while being continuously dragged by the near-surface hydrodynamic flow, allowing us to finely disentangle chain/wall and chain/solvent frictional molecular interactions. By allowing for direct observations of molecular-scale interfacial dynamics, our approach brings a new molecular vision of macromolecular friction and adsorbate/surface interaction at flowing solid/liquid interfaces.

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Keywords: macromolecules, dynamic, microscopy, adsorption

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[*] Speaker

Colloidal Nanoparticles, Nanowires, and Nanosheets: From Synthesis to Applications

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Solution-processed semiconducting nanomaterials, including colloidal nanoparticles, nanowires, and nanosheets, present an exciting avenue for next-generation optoelectronic devices. Their optical and electronic properties can be finely tuned by adjusting their size and shape, making them suitable for a variety of applications such as solar energy harvesting and advanced photodetectors. The ability to modify these properties through simple chemical processes has spurred significant research into their use in photovoltaic technologies.

The first part of this thesis addresses the stability issues associated with PbS quantum dot (QD) solar cells. Despite their promising broad absorption spectrum and tunable bandgap, these cells face challenges related to the stability of the PbS-EDT (1,2-ethylenedithiol) hole transport layer (HTL). While initial exposure to oxygen may enhance performance by improving electron-blocking, prolonged exposure results in the oxidation of the PbS-EDT layer, leading to decreased efficiency. This instability is a barrier to achieving long-term performance. To counter this, we investigate novel HTL molecules developed at Cergy Paris Université-HL36, HL37, HL38, and HL39-that have shown promise in perovskite solar cells. While PbS-EDT remains more efficient, HL39 emerges as a viable alternative, and devices using HL38 and HL39 demonstrate improved stability in air, suggesting a path toward more durable PbS QD solar cells.

The second part of the thesis examines the use of low-dimensional perovskite nanosheets in phototransistors. This research aims to meet the demand for lightweight, multifunctional optoelectronic devices by integrating perovskites with materials like graphene, known for its high charge mobility but limited optical absorption. We focus on achieving a homogeneous thin film of quasi-2D perovskite with the formula PEA2Csn-1PbnBr3n+1 and exploring its optical properties. Future work will involve combining this with graphene in a field-effect transistor (FET) architecture to investigate the optoelectronic and electroluminescent properties of these hybrid devices.

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[*] Speaker

In-situ Interfacial Temperature Evolution of Perovskite Solar Cells Over Degradation Measurement Achieved by Up-conversion nanoparticles

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The instability of PSCs remains a significant challenge, as they tend to degrade upon exposure to environmental factors, such as ultraviolet (UV) radiation, oxygen, humidity, and temperature. The origins have been linked to halide segregation, ion migration, and decomposition. In previous studies, various environmental factors have been often treated as independent variables while the evolution of the solar cells' PCE was monitored so that different engineering approaches can be identified to mitigate the undesirable instability of PSCs. However, during PSC degradation, apart from the macroscopic device performance, other properties of the different layers involved and their interfaces also undergo continuous changes, such as material composition and their optical properties (e.g. absorption and photoluminescence (PL)), leading to changes in the electrical properties and thermal environment of the device. In this work, we introduce a novel local electro-optical scanning technique to monitor in-situ temperature fluctuations, photoluminescence (PL) intensity, and changes in power conversion efficiency (PCE) of two distinct compositions of PSCs (FA0.9MA0.1PbI3 & FA0.87MA0.13PbI2.87Br0.13) at the nanoscale during degradation. This method leverages inorganic Er3+ doped NaYF4 colloidal nanoparticles. To the best of our knowledge, this is the first instance where the correlation between nanoscale temperature elevation inside solar cells and degradation has been experimentally unveiled.

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*Speaker

GRAIN DISPERSION IN GRANULAR FLOWS

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Mixing is crucial in industries like glass and concrete manufacturing, where inadequate homogenization affects the final product quality. Chaotic flows enhance mixing at low Reynolds numbers due to the mechanisms of advection and diffusion, whose respective contributions can be quantified by the Péclet number (Aref, 1984). Fluid mixing can be quantitatively analyzed via concentration fields (Villermaux, 2019). Despite extensive studies on fluid mixing, granular mixing in smooth flows is less understood, complicated by factors such as the discrete nature of grains and the lack of thermal agitation (Ottino & Khakhar, 2000). We developed a 2D dry granular experiment in a closed setup, using a figure-eight protocol to stir the grains. By tracking individual grains, we quantified the separation of Lagrangian trajectories and the dispersion of tagged particles toward homogeneity. In particular, we focused on the change in mixing rate produced by regularly rotating the axis of the figure-eight pattern. Our results suggest potential improvements in dispersion models for smooth granular flows through further analysis of variance decay. Ongoing Discrete Element Modeling (DEM) simulations aim to characterize the Péclet number for granular flows and to explore the dependence of the mixing process on this parameter.

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*Speaker

Design of innovative bio-based and biodegradable hydrogels from itaconic acid

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Hydrogels are 3D cross-linked polymer networks capable of retaining significant amounts of water within their structure and still have the properties of solid materials. Hydrogels materials have been increasingly studied and developed for various applications. Initially employed in hygiene products, their use has expanded to include food packaging, agriculture applications and even chemical sensors. Hydrogel also find applications in biomedicine, thanks to their swelling properties. However, most of these commercial hydrogels are petroleum-based and non degradable, resulting in serious environmental concerns.To overcome these limitations, various natural polymers have been used as potential substitutes for petroleum-derived synthetic hydrogel. Even though they are bio-based and biodegradable, the high molar mass of these polymers complicates the control of their architectures. Additionally, they often require grafting with petroleum-derived monomers to achieve desired swelling properties. In this context, we developed fully biobased and biodegradable hydrogels using itaconic acid, a biobased monomer extracted from Aspergillus terreus fungi. Itaconic acid was used to form the hydrophilic polymer network but also to synthesize novel biobased cross-linkers, offering a renewable and eco-friendly alternative to traditional petrochemical acrylates. These gels were stable in water, with an outstanding water capacity, exceptional swelling behavior, and robust mechanical properties. These properties were evaluated for different hydrogel formulations as well as under various conditions (pH and ionic strength). A detailed study was conducted to examine the behavior and optimize the properties of these hydrogels, aiming to improve their performance for a wide range of potential applications. It has been demonstrating that the specific interactions within the polymer matrix are responsible for superior physico-chemical and mechanical properties. Gaining a deeper understanding of the structure-property relationship of these hydrogels is intended to further enhance their performance for various potential uses. Furthermore, ultimate biodegradability tests were conducted on various hydrogel formulations, highlighting their biodegradation potential.

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*Speaker

Synthesizing and characterizing a new class of star polymers based using pillararenes as initiator for anionic ring-opening polymerization

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Liposomes have served as basic models for mimicking the compartmentalization and selective permeability of natural cells. However, their mechanical stability limitations have spurred the development of synthetic analogs, called polymersomes1. These vesicles, formed from amphiphilic block copolymers, offer enhanced stability and versatility in applications like drug delivery and nanoreactors.
This project aims to develop biomimetic polymersomes thanks to amphiphilic copolymers2, synthesized with poly(butylene oxide) (PBO) hydrophobic blocks and polyglycidol (PGL) hydrophilic blocks.

A series of triblock copolymers PGLn-PBO2m-PGLn and pillar(5)arene3,4-based star copolymers PIL-(PBOm-PEEGEn) were synthesized through sequential anionic ring-opening polymerization using pillar(5)arene derivative as initiator, subsequently hydrolyzed to provide the PIL-(PBOm-PGLn) as described in scheme 1.

The structures of the copolymers were characterized by NMR and size exclusion chromatography (SEC). Thin-film rehydration technique was then used to prepare the self-asssemblies of the copolymers in solution. The morphology of the self-assembled polymers were systematically investigated by dynamic light scattering (DLS), static light scattering (SLS), small angle X-ray scattering (SAXS) and cryo- transmission electron microscopy (TEM).

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*Speaker

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The results reveal that by adjusting the weight fraction of PGL (WPGL), the copolymers transition from small, spherical micelles at low WPGL to worm-like micelles and to large, hollow polymersomes at higher WPGL. The permeability5 of the polymersomes is under investigation, in order to use the nano-objects for encapsulation and release purposes.

Keywords: Amphiphilic Copolymers, Polymersomes, Pillararene

Ternary titanium oxides: superionic conductors

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A significant amount of research has focused on developing new energy storage devices with longer lifespans and greater energy capacity. Recently, significant interest has been in finding alternative energy storage technologies that rely on non-critical mineral resources. Additionally, there has been increasing focus on solid-state batteries in order to enhance the conductivity and stability of the energy storage devices.

Certain ternary titanium oxides of the Andersson-Wedsley family with the following chemical formula (M2Ti2O5), such as Rb2Ti2O5 (RTO) and K2Ti2O5 (KTO), exhibit a high ionic conductivity (σ(RTO) = 0.1mS.cm–1 and σ(KTO) = 0.01mS.cm–1) at room temperature. These oxides also demonstrate a colossal equivalent dielectric permittivity at room temperature, making them good candidates as super-capacitors.
These materials are single-crystals that exhibit a strong hygroscopic behaviour, which directly influences the conductivity and the dielectric properties of these materials. Numerous experimental techniques have been used to study these materials in order to understand the effects caused by incorporated water molecules on the physical and chemical properties of RTO and KTO. The crystallographic structure of RTO and KTO with different water contents has been investigated with Transmission Electron Microscopy (TEM) and Scanning Electron Microscopy (SEM).
RTO and KTO also demonstrate a complex local electrostatic charge distribution that was investigated with the Pressure-Wave-Propagation method (PWP). This method shows negative charge accumulation at the anode and an insulator-metal transition at the cathode. A new experimental method that couples cyclic voltammetry to the PWP (CV-PWP) method was developed in order to help study this complex electrostatic charge dynamic. This operando method probes some chemical and physical information during charging-discharging cycles.
In conclusion, extensive research has been concentrated towards the development of solid-state batteries utilizing non-critical mineral resources. Single-crystals of RTO and KTO have demonstrated promising ionic conductivity and remarkable dielectric permittivity, making them interesting candidates as solid electrolytes.

Keywords: solid electrolyte, titanium oxides, ionic conductivity, electrostatic charges

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*Speaker

Dynamics of 2D ribbons in liquid crystals topological defects

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Smectic liquid crystals (LCs) exhibit various topological defects (TDs) where nanoparticles can be confined and organized. It has been shown that confinement induced by smectic patterns, made up of oriented ribbon-like grain boundaries (2D topological defects), leads to the formation of oriented ribbons of fluorescent nanorods. My thesis investigates the dynamics of these nanorod assemblies within smectic TDs, where the particle dynamics often deviate from typical Brownian diffusion.

My work aims to better understand the confinement-induced dynamics in smectic TDs, as structural information about the smectic defect matrix can be indirectly inferred, and active control of nanorod assembly structure may be possible through their dynamics. Using optical microscopy, fluorescence microscopy, and synchrotron-based grazing incidence X-ray scattering (GISAXS), we reveal a unidirectional motion of the nanorod ribbons along the defects, confined strictly within the smectic structures. This motion includes small-scale fluctuations and jumps between two equilibrium positions. This behavior is similar to subdiffusive dynamics observed in particles confined in polymer networks, showing that the motion of the nanorod assemblies in the smectic defects is trap-like.

The size and density of the nanorod assemblies influence the fluctuation and jump values, indicating that smectic elasticity, induced by the presence of the nanorods (larger than the defect core), drives these dynamics. This allows us to precisely measure the smectic distortion caused by each nanorod assembly and the spatial variation of these distortions, which depend on the organization of the nanorods.

We demonstrate that increasing the temperature near the smectic/nematic phase transition eliminates this subdiffusive behavior, inducing continuous diffusive motion. This allows the ribbons to elongate up to 10 micrometers, potentially enabling future studies on the transport properties of nanoparticle ribbons, such as connecting electrodes with single ribbons.

Keywords: liquid crystals nanoparticles self, assembed diffusion

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[*] Speaker

Control underwater bioadhesion with surface topography and molecular interactions

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Adhesive in aqueous environment has been one of the topics that gain more attention. The water screening effect between the interface of adhesive and substrate tremendously reduced adhesion efficiency resulting in the restriction of adhesive in submerge applications. While significant experimental and theoretical advances have been made on adhesion of synthetic materials,1 there is still a clear lack of knowledge on more complex bio-adhesion processes in wet conditions. This can be addressed by a systematic design of bio-based adhesives with controlled and variable surface topography, chemically active interactions and viscoelastic properties.

In this work, mechanisms and factors affecting underwater adhesion were studied using homemade probe tack test which enables to finely characterize the underwater adhesion properties between a tough hydrogel adhesive and solid substrates modified by hydrogel macro- and micro-patterns. This configuration allows to separate the effect from bulk (cohesion) and surface properties. 2 Macroscopic tough bio-based double network (DN) hydrogels with negative charges of -carrageenan/agarose and poly(acrylamide) were developed. Model hydrogel thin films (_˜100 nanometre) and microscopic hexagonal hydrogel patterns with positive charges poly((dimethylamino)ethyl methacrylate) (PDMAEMA) were prepared via cross-linking and grafting (CLAG) strategy using photolithography technique.3 The effect of aqueous environments and surface topography by changing hexagonal side length (20 and 200 micrometre) and distance between hexagon patterns (20 and 200 micrometre) on adhesion energy were investigated.

We measured adhesion energy between PDMAEMA hydrogel thin film and tough DN hydrogel about 8.5 J/m2 as a result of strong positive-negative charge interaction. The contribution of the surface topography to the adhesion energy was also showed. A significantly increased adhesion energy from 8.5 to 37 J/m2 could be observed for the underwater with hydrogel micropatterns as a result of the water drainage effect and the crack propagation preventing from the hexagonal patterns.

Keywords: underwater adhesion, bioadhesion, biopolymer, hydrogel

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*Speaker

Decoding madder dyes through computational chemistry

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Unlike synthetic dyes, which produce a single hue, natural dyes reveal a rich spectrum of colors. Traditionally, artisans have relied on a lifetime of expertise to control these shades. With advancements in computational chemistry, predicting dye colors from UV-Vis spectra has become more precise and efficient. However, most existing studies focus only on the spectra of individual molecules. However, natural dyes consist of complex mixtures, unlike the pure compounds used in synthetic dyes. To address this gap, we have developed an innovative computational method to predict the spectra and color of plants containing multiple dye molecules. Our study centers on Madder, a historically significant dye plant used in textiles and pigments. We measured the concentration of the primary molecule using Liquid Chromatography-UV-Mass Spectra (LC-UV-MS/MS). The computed spectra were generated using Time-Dependent Density Functional Theory (TD-DFT), the Adiabatic Hessian and the Vertical Gradient framework and then converted into CIELAB color coordinates. Our method shows exceptional accuracy, with predicted spectra differing from experimental results by less than 0.2 eV, within the standard error margin for DFT-based methods. It offers excellent convergence and is flexible enough to handle a broad range of molecules, including those with large sugar moieties.

Keywords: Computational chemistry, dyes, madder, UV, Vis spectra, color

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*Speaker

Mechanics in shear of waterborne Pressure Sensitive Adhesives (PSAs) based on vitrimer chemistry

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Pressure sensitive adhesives (PSAs) are ubiquitous and there is already expertise on how to enhance their adhesion performances. Yet the possibility of easy and controlled debonding is now of high interest for disassembly process, in the context of sustainable development.
The VITRIPSA ANR project aims at synthesizing a new generation of water-based PSAs from vitrimer-like particles. After short annealing times, dynamic bond exchanges at interfaces should connect the crosslinked particles together forming a nanostructured film with good overall mechanical and adhesion properties. More extended annealing at higher temperatures could provide extensive interdiffusion between nanostructured domains to reach phase randomization and de-adhesion. Hence, high-performance adhesives can be obtained with unprecedented control over the structuration and viscoelastic properties, with the possibility of heat-deactivation of the adhesion.

My approach will be focused on the characterization of the adhesive properties of these model materials, especially their resistance to shear over long times and low loads, a poorly understood property.
I will present our analyses on PSAs deformation under shear with a custom-designed lap shear testing device. A parametric study has also been completed examining how the non-linear rheology affect adhesion of PSAs under shear.

Keywords: Adhesive, shear, vitrimer

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*Speaker

Tuning self-assembly of hydrophilic polymers in water through an aromatic supramolecular structure directing unit (SSDU)

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The self-assembly of hydrophilic polymers in water can be driven using different strategies, the most common being the introduction of hydrophobic groups to the chain end(s)(1). To obtain anisotropic or more complex assemblies, so-called supramolecular structure directing units (SSDU) have been designed and introduced in the center or the chain end of hydrophilic polymers.(2) Recently, our team showed that the functionalization of a RAFT agent by a bis-urea SSDU allows the production of polymers that self-assembly in water into nanocylinders, via unidirectional hydrogen-bonding of the terminal bis-urea sticker(3).

The objective of our work was to develop a simple and direct method to obtain anisotropic nano-objects in water making use of the directional supramolecular π-π interactions of a perylene diimide sticker incorporated in the core of hydrophilic polymer chains(4). Surprisingly, simple addition of water to the polymer powder was sufficient to dissolve all polymers synthesized. For the shortest polymers, nanoribbons were obtained driven by the assembly of the PDI units in a combination of H- and J-type PDI aggregates. The formation of these 2D assemblies was followed over time by UV-VIS absorption spectroscopy, cryo-TEM and SAXS. UV-VIS enabled us to identify the different types of aggregates present in the assemblies. Finally, upon temperature increase a quasi-reversible transition between ribbons and cylinders was observed by cryo-TEM, which was explained on a molecular level by the loss of J-type aggregates.

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*Speaker

Keywords: Perylene diimide, Supramolecular Structure Directing Unit, Self, assembly, Anisotropic nanostructures, Structure, property relationship

Synthesis of New Glycine-Based Polymers and their Thermoresponsive Behavior in Water

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In recent years, polymers possessing an Upper Critical Solution Temperature (UCST) in water have raised a growing interest due to their potential application in smart systems for biomedical applications.(1) Hitherto, only a few examples of neutral UCST polymers in water has been reported in the literature.(2) In this context, our group has developed a new family of polymers based on *N*-cyanoalkylacrylamide monomers. Some of them possess an UCST behavior in water, whereas others exhibit LCST-like transitions or are not thermoresponsive.(3,4) During my PhD thesis, a series of novel monomers containing one, two, or three amide functional groups and one terminal cyanomethyl group was synthesized. In this case, all resulting homopolymers, obtained by free radical polymerization (FRP) and reversible addition fragmentation chain transfer (RAFT) polymerization, display a sharp and reversible UCST-type phase transition in water. We have shown that the cloud point (TCP) can be adjusted over more than 60○C by the number of glycyl groups present in the monomer structure and by the polymer's molar mass.(4)

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Keywords: RAFT Polymerization, UCST, water, soluble thermosensitive polymers

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[*] Speaker

Coupling Photostriction and Magnetism in Vertically Assembled Nanostructures

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Vertically aligned nanocomposites (VAN) constitute a well-suited system to study the coupling effect between photostriction-photoinduced non-thermal expansion-in SrRuO3 (SRO) and inverse magnetostriction-deformation under a magnetic field-in cobalt ferrite CoFe2O4 (CFO). The VAN system consists of a thin film made up of a network of nanowires (CFO) perpendicularly embedded within a matrix material (SRO), all in epitaxy. The architecture of the VAN not only promotes perpendicular anisotropy due to the cylindrical shape of the magnetic inclusions but also enhances the multiferroic coupling effect by maximizing their surface-to-volume ratio. The nanocomposite system has been synthesized using pulsed laser deposition (PLD) and analyzed in its crystallographic structure, magnetic anisotropy, vibrational properties and morphology using X-ray diffraction, vibrational sample magnetometry (VSM), Raman spectroscopy and atomic force and electron microscopies (AFM, SEM, TEM).

Keywords: magnetism, thin films, photostriction, magnetostriction, ferrites, nanocomposites, epitaxy

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*Speaker

Aqueous foams for the leaching of micrometric copper particles

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Aqueous foams are an interesting medium to perform heterogeneous chemical reactions, as they combine liquid and gaseous reactants, while minimizing volume of aqueous effluents. We thus showed that foams are an efficient medium to oxidize metals such as copper and silver, whose oxidation relies on fast oxygen transfer. (1-3) In the present work, we study the oxidation of micrometric copper particles, as reference for the particles typically encountered in the recycling process of electronic wastes that we plan to target. We disperse these particles within a rotating foam whose liquid phase contains an acidic reactant, and whose gaseous phase contains the oxidant, namely oxygen in air. We show that the rotating speed is a crucial parameter to control both the foam effective liquid fraction and the reactants repartition within the foam. Focusing on reactants transport, we also show that the liquid fraction of the foams should be tuned depending on acid concentration, in order to favor either oxygen transfer as it is the case for dry foams, or protons and particles displacement, as it is the case for wetter foams.

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*Speaker

Keywords: foams, oxidation, metallic particles, leaching

Cross-linking mechanisms in elastomer blends: relationships between morphology, cross-linking heterogeneities and mechanical behaviour

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Elastomer blends composed of Natural Rubber (NR) and Butadiene Rubber (BR) are key materials widely used in the automotive/tire industry and more precisely, in the design of tire treads and anti-vibration materials. High mechanical performances (wear resistance, tire grip and braking) are indeed obtained by blending NR with BR**1**.
For immiscible or partially miscible NR/BR blends, the solid-state organization of the different phases significantly affects the mechanical properties of the final materials, such as the elastic modulus or the crack resistance. The extent of cross-linking in each blend phase is also crucial since it should significantly influence the elastic behaviour of the blends. However, this feature has been poorly addressed from an experimental point of view, due to the lack of selective experimental methods allowing to investigate the distribution of the cross-link density within each kind of domains. In this context, this work aims at examining cross-linking heterogeneities in NR/BR elastomer blends in order to get a better understanding of the process conditions needed to achieve specific elastic properties for the final materials.

The morphology of cross-linked NR/BR blends was analysed using contrast-phase optical microscopy, DSC and 1H solid-state NMR (1H T1 relaxation). In a second step, 1H double-quantum based NMR experiments**2** were used to determine the distribution of the cross-link

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density in NR-rich and BR-rich regions. Finally, uniaxial tensile tests were performed and the data obtained at the macroscopic level will be correlated to the blend morphology on the one hand and the distribution of the cross-link density on the other hand.

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Keywords: elastomers, dynamics, cross, linking, heterogeneities, structure, property relationships, natural rubber

Ni exsolution from (NiO)x(ZrO2)1-x for catalytic CO2 valorization

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Nickel (Ni)-based catalysts have gained significant attention due to their abundance, affordability, and robust performance in CO2 transformation processes, making them attractive candidates for sustainable CO2 utilization technologies such as methanation and reverse water-gas shift (RWGS), with a realistic potential for large-scale deployment. Among the supports studied for CO2 valorization, zirconia (ZrO2) stands out due to its excellent thermal stability and mechanical strength, as well as its CO/CO2 adsorption capability. Here, a phenomenon widely studied in perovskites will be applied in the preparation of Ni-ZrO2 catalysts, namely exsolution. It represents a novel approach to catalyst synthesis which results from the metal ion migration within the hosting support towards the surface, often under reducing atmospheres. The exsolution generally provides superior control over particle size, a high content of well-dispersed metal, and strong metal-support interactions, with the anchoring of the metal making catalysts more resistant to sintering, thereby optimizing catalytic performance and extending catalyst lifespan.

The objective of the present work is to explore exsolution of (NiO)x(ZrO2)1-x mixed oxides prepared by co-precipitation, particularly focusing on the reduction conditions and structure-exsolution relationships, in order to optimize the dispersion/size of exsolved Ni nanoparticles, and thus the catalytic performance in CO2 hydrogenation at atmospheric pressure.

The *in situ* XRD results confirmed the feasibility of Ni exsolution in the (NiO)x(ZrO2)1-x material, which exhibits high NiO dispersion and a relatively high specific surface area (_˜80 m^2/g) at relatively low temperatures (500-600 $\circ$C) with extended durations, without significantly reducing the specific surface area. The material was investigated as a CO2 methanation catalyst, and it was observed that CO is predominantly produced following the exsolution process. The current work focuses on elucidating the mechanism of the material after exsolution in CO2 hy-

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drogenation. This valuable finding could potentially open up new opportunities for utilizing this catalyst in the RWGS reaction.

Bio-detection using Whispering Gallery mode enhanced Energy Transfer (WGET) sensors excited by fluorescent nanocrystals

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Fluorescence-based biosensors have attracted much attention in the domain of biomedical diagnostics thanks to their high specificity, ease of use and fast response. One of the worth noting fluorescence assays is based on Förster resonance energy transfer (FRET) due to its multiple advantages as a rapid, easy to use and highly specific analysis. However, this technique has a strong dependence on the donor-acceptor distance (_˜ 10 nm), which limits the sensitivity. To overcome this limitation we introduce a novel highly sensitive biosensing platform based on optical microcavities with high quality resonance modes (whispering gallery modes, WGMs) as an energy donors. These resonances generate an evanescent field, which spreads up to a few tens of nm outside the cavity surface. When a biomolecule is placed at the surface of the cavity, it interacts with this evanescent field, which leads to a spectral shift of the resonance. Several studies have demonstrated that this allows the detection of analytes with small concentration and with different range of sizes. However, the detection of this spectral shift requires advanced spectroscopy tools. Here, we propose a new generation of easy-to-use biosensors based on whispering gallery energy transfer (WGET) using quantum dot-loaded spherical microspheres supporting high quality WGMs as donors and organic dye-loaded nanoparticles as acceptors. This assay gathers the high specificity and simplicity of FRET and the high sensitivity and long-range sensing ability of WGM cavities. We first demonstrate a simple WGET assay, where biorecognition between acceptors and the microsphere donors are mediated by biotin-streptavidin interactions, with a typical sensitivity in the fM range. Then, we explore the possibilities of using WGET in the detection of biomarkers using oligonucleotide- (DNA)- mediated recognition.

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*Speaker

Keywords: Energy transfer, Quantum dots, Biodetection

Synchrotron-based electronic characterization of organic thin films for non-fullerene acceptor solar cells

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The transition from fullerene to non-fullerene acceptors (NFAs) has drastically increased the power conversion efficiency (PCE) of organic photovoltaics, reaching PCEs above 19% (1). As opposed to fullerene acceptors, NFAs have tuneable energy levels, stronger absorption across the solar spectrum, and better thermal stability. The PM6/Y7 polymer donor/NFA binary blend is one of the most promising systems (2) thanks to its broad absorption range, which favors high photocurrents in such based devices (3). Frontier orbital band alignment is a key factor affecting the device's efficiency. This aspect remains unexplored in the PM6/Y7 blend system, especially with varying donor-acceptor ratios.This work aims to investigate the electronic structure and the energy band alignment of spin-coated PM6/Y7 thin films on a ZnO substrate, by studying the evolution of the core levels, the work function, and the frontier orbitals (valence and conduction bands) as a function of the different ratio between the donor and acceptor molecule in the blend. To obtain this energetic landscape, we employed synchrotron techniques such as X-ray photoemission spectroscopy, which allowed us to access the core levels, UV photoemission spectroscopy for determining the work function and the HOMO onset, and X-ray absorption spectroscopy to get the LUMO onset. From these measurements, we observed a decrease in the transport bandgap from the neat molecules to the 1:1 blend and a further decrease when transitioning to the 1:2 and 2:1 blend (Fig. 1). However, from the energy band alignment, we

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*Speaker

observed a non-optimal donor/acceptor behaviour for charge extraction, which, on the other hand, improves significantly using a gold substrate. In summary, we have taken a significant step forward in understanding this efficient, unexplored system by observing electronic structure changes between the pure molecules and the blend and by obtaining a picture of its energy band alignment.

Keywords: non, fullerene acceptors, organic photovoltaics, energy band alignment, electronic structure, X, ray photoemission spectroscopy

Nanoscale hydrophobicity of a macroscopically hydrophilic surface: hydroxylation kinetic of siloxanes in aqueous medium studied by force spectroscopy

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Silicon dioxide (SiO) is a compound that exists in various forms, both crystalline and amorphous, and can be naturally found as quartz (100), the second most abundant mineral on Earth. Its behavior in contact with aqueous solutions has been extensively studied and is one of the primary keys to understanding the physicochemical phenomena that occur, such as dissolution and adsorption processes, especially in the context of the geochemical origins of life. These processes depend on the surface chemistry of silica, determined by its relative composition of silanol (Si-OH) and siloxane (Si-O-Si) groups. Silanol and siloxane groups exhibit significantly different hydrophilic and hydrophobic properties: silanols form hydrogen bonds with water molecules and contribute to the well-known hydrophilic nature of silica surfaces in the literature. Siloxane groups, on the other hand, although polar, are largely considered hydrophobic sites. One widely used technique to probe the relative hydrophobicity of a surface is contact angle measurement. However, this technique provides an ensemble-average estimation of the hydrophobicity of the surface, which demonstrates an overall hydrophilicity of silica surfaces. Using atomic force microscopy (AFM)-based force spectroscopy, this study focuses on the nanoscale investigation of hydrophobic sites of macroscopically hydrophilic silica and presents the hydroxylation over time of surfaces initially covered with siloxane sites. The hydroxylation kinetic is studied by force spectroscopy and compared with contact angle measurements. Further single-molecule force spectroscopy (SMFS) measurements carried out using a hydrophilic peptide revealed not only the presence of siloxane patches on silica surfaces but also a difference in the reorganization of these patches after rehydroxylation, depending on the thermal treatment received.

Keywords: Silica, Hydroxylation, Force spectroscopy, Hydrophobicity, Origin of life

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[*] Speaker

Chiral CdSe nanoplatelets for strong chiro-optical features

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II-VI semiconductor nanoplatelets (NPLs) have recently arisen as an enhanced version of spherical quantum dots (QDs), where improved optical features emerge from the flat geometry and subatomic roughness. In order to implement strong chiro-optical features, we propose a post-synthetic ligand exchange with tartrate ligands on CdSe NPLs. Surprisingly, the exchange undergoes several stages, with an increase of the Circular Dichroism feature at the position of the heavy hole, followed by an inversion of the signal when the absorption saturates. The dissymmetry factor can reach values as high as 1.2 x 10-2.

The peak inversion global aspect is influenced by the lateral aspect of the initial particle, the former surface chemistry, and the synthesis conditions. It is attributed to a mechanical relaxation of the system, that induces a stress-dependent coupling between the inorganic core and the chiral ligand. This hypothesis is supported by surface chemistry characterization and XRD analysis.

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[*] Speaker

4D printing of objects exhibiting magnetic and plasmonic responses

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Additive manufacturing is becoming a key technique to create complex objects. However, a need to expand its possibilities is emerging. 4D printing has come to light in this context by combining smart materials with additive processes to create stimuli responsive 3D printed objects. For example, magnetism is usually used to induce actuation of a printed unifunctional piece, by using the properties of a polymeric matrix charged with dispersed magnetic particles. In this project, we aim at developing 4D printed multifunctional objects based on the combination of a functional matrix embedding multi-elemental fillers, nano and microstructured gold-magnetite assemblies. The objective is to obtain designed magnetoplasmonic active elements, responsive to light and magnetic field.

First, a scale-up synthesis of raspberry like magneto-plasmonic nanoparticles was developed and particles were obtained by functionalizing magnetite particles with gold nanoparticles, giving 400 mg of particles per synthesis, enabling the production of a sufficient quantity of particles for printing. Secondly, we investigated the incorporation into a homemade photo-polymerizable resin for 3D printing by Digital Light Processing (DLP). The object is printed under a magnetic field to assemble the nanoparticles into microstructures in chain like shapes.

This strategy allows the printing of magneto-responsive objects, able to actuate by the application of an external magnetic field. And, as the self-assembled chains are formed of raspberry like magneto-plasmonic nanoparticles, hot spots between gold nanoparticles can be used to add a second functionality to the object. The optical properties and local arrangements of nanoparticles have been analysed by hyperspectral microscopy. The printed systems showed strong photoheating, thanks to gold nanoparticles, modulated by the wavelength and the intensity of the light source.
Finally, these 4D printed magneto-plasmonic elements open intriguing perspective to design unprecedented 4D printed devices such as programmable optical sensors.

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*Speaker

Enhanced THz signal from Spintronic Emitters with integrated metallic cavities

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The Terahertz domain is the region of the electromagnetic spectrum ranging between 0.1 and 10 THz (30 μm $< \lambda <$ 3 mm), in between the Infrared and the microwave region. THz can be exploited for different applications such as medical imaging, astronomy, or wireless telecommunications. More specifically, THz can be used in solid state physics to probe matter at the picosecond timescale unveilling information such as the dynamic of free-carriers and phonons or magnetization processes. The need for efficient and broadband THz sources is therefore crucial for material caracterization through THz spectroscopy.

Spintronic Terahertz emitters (STEs) based on optical excitation of nanometer thick ferromagnetic/heavy metal (FM/HM) heterojunction are THz broadband pulsed sources, which makes them promising for spectroscopy applications. However, the efficiency of the optical-to-THz conversion remains limited compared to other more mature THz technologies. To answer to this problematic, the aim of this work is to enhance the state-of-the-art efficiency of STEs with photonic control of the emitted THz pulses through structure engineering.

Therefore, to enhance emission in a selected THz spectral range, FM/HM structures are realized on ultra-thin sapphire layers with metallic mirrors to create $\lambda/4$ THz resonant cavities. The THz emission is caracterized with the THz emission time domain spectroscopy (TDS) technique, that allows to reconstruct the temporal profile of the Electric Field with a highly resolved femtosecond precision. Cavities with thicknesses of a few tens of microns are investigated, displaying up to a doubling of the field in the spectrum of emission. Experimental results are compared to simulations modelling the system and predicting an even further improvement of THz efficiency using thinner cavities.

Keywords: Terahertz, Spintronique, Optique ultrarapide, Spectroscopie terahertz

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*Speaker

Fast Electrodeposition of Iron rich NiFe-LDH contains Fe2+ for Enhanced Oxygen Evolution Reaction: A Direct Path to Design Active and Durable Electrocatalysts.

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In this study, we utilized a rapid ($t < 1$ min) electrosynthesis technique, using Fe2+ ions to form the NiFe-hydroxide, followed by partial iron oxidation to generate the NiFe-LDH. This approach effectively incorporates iron into the structure without forming the inactive phases and also maintains a Fe2+ component within the NiFe-LDH structure (**Fig.1a**). We explored the effect of electrodeposition potential and the Ni/Fe ratio in the solution to identify the optimal iron content for enhanced OER performance. Scanning electron microscopy (SEM) revealed that iron-rich NiFe-LDHs exhibit a nanosheet array morphology, with aggregation on the surface influenced by both the applied potential and the metal ion concentration. At potentials below -1V vs. Ag/AgCl (3M KCl) and with Ni/Fe ratio in solution > 1, vertically standing nanosheet arrays were formed. At higher potentials and with Ni/Fe ratio in solution < 1, nanosheet clusters resembling sand roses appeared on top of the arrays. Increasing the cathodic electrodeposition potential led to more clusters and a higher Ni/Fe ratio in the film. X-ray photoelectron spectroscopy (XPS) indicated an increase in Fe3+ with increasing electrodeposition potential, maintaining a constant M3+/M2+ ratio of 0.36, consistent with the hydrotalcite structure. Cyclic voltammetry (CV) and linear sweep voltammetry (LSV) demonstrated the influence of iron content in film on the shift of oxidation/reduction potentials for Ni. The NiFe-LDH synthesized at -2.0 V vs. Ag/AgCl (3M KCl) with 55 atomic % iron (Ni/Fe = 0.78 in film) exhibited overpotentials of 192 ± 10 and 234 ± 8 mV at 10 mA.cm-2 and 30 mA.cm-2, respectively (**Fig.1b**). Furthermore, it stable for 100 hours of operation at 100 mA.cm-2 and maintained its morphology without change after stability test (**Fig.1c**), demonstrating exceptional activity and stability among NiFe-LDH catalysts with high iron content. This highlights the effectiveness of the electrodeposition method (via hydroxide oxidation) in producing low-cost, iron-rich LDHs.

Keywords: Electrodeposition, Hydroxide, Layered Double Hydroxide, iron rich, Oxohydroxide,

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*Speaker

Oxygen evolution reaction.

Development of Orientation-Patterned Gallium Phosphide based photonic devices for spectral translation of optical frequency combs

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Many applications, such as spectroscopy (1), require frequency combs centered in the visible. Technologically mature combs are centered around 1.55 μm. The conversion of these combs from infrared to visible using nonlinear optics is a promising way to overcome this bottleneck. Due to its intrinsic properties, such as high nonlinear coefficients of order 2 and 3 and a wide transparency range (0.5 - 12 μm), orientation patterned gallium phosphide (OP-GaP) is of particular interest in integrated photonics for the conversion of frequency combs to the visible: in periodic patterns, OP-GaP allows efficient spectral translation from a telecom frequency to the visible (2). However, the bandwidth of the converted spectrum remains limited to a small range centered around a main frequency. In this paper, we propose to modulate the spectral response of the OP-GaP by broadening the conversion bandwidth of the device in order to obtain an optimal translation from the C-band to the visible. To this end, numerical simulations have been performed to compare two OP-GaP waveguide designs, namely a periodic pattern and a chirped pattern. An optimization criterion was established to guide the fabrication of OP-GaP waveguides for comb translation, which is currently ongoing.

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Keywords: Gallium Phosphide, Suspended Waveguide, Nonlinear Optics

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*Speaker

Interfacial self-assembly between polydiacetylene and graphene oxide and the formation of silver nanostructures by X-ray-induced water radiolysis.

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My PhD research involves two steps. The first step is to form and study the interface between a polydiacetylene (PDA) and graphene oxide (GO) for optoelectronic applications, such as solar photovoltaic. The appealing optical and conductive properties of this hybrid system rely on the organization between GO and PDA at the interface. I use the Langmuir procedure to form the interfacial assembly on a liquid matrix. I deposit GO sheets and diacetylene (DA) monomers on a water surface. Their amphiphilic properties make them stay on the surface of the water and not sink. I compress the two species and eventually, one is expected to climb over the other one, forming the interface. Then, I photopolymerize the diacetylene monomers to obtain the desired assembly of GO and PDA. I first study the mixed GO/DA system directly on the liquid subphase (before polymerization) by Π-A isotherms, Brewster Angle Microscopy, and X-ray scattering techniques using a synchrotron source. Then, after polymerization, I study the optical properties of the hybrid film by UV-VIS absorption. Eventually, I transfer the GO/PDA mixed film onto a solid substrate for Atomic Force Microscopy, Kelvin Probe Force Microscopy, RAMAN, and X-ray Photoelectron Spectroscopy. The second step is to anchor a silver (Ag) film to the GO/PDA assembly. Indeed, the final goal would be a system based on GO, PDA, and Ag, with appealing flexibility, transparency, and conductivity for solar cell applications. The GO/PDA assembly is formed on an aqueous subphase that contains a silver salt, and it is irradiated by synchrotron-sourced X-rays at an incident angle below the total reflection. This results in a film of reduced silver atoms anchored below the GO/PDA system. The X-ray beam not only induces the radiolysis process but also enables in-situ diffraction and fluorescence experiments to further characterize the final system.

Keywords: Soft, matter, Langmuir Films, Graphene Oxide, Polydiacetylene, Polymerization, Synchrotron, sourced X, rays, Silver Nanostructures, Water Radiolysis

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*Speaker

Exploring heat generation in layered oxide Na-ion 18650 cells using optical calorimetry

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The development of commercial sodium ion batteries requires high-performance cathode materials. Due to their high specific capacity and low environmental impact composition, layered oxide materials crystallized in P2 and O3 phases are highly promising contenders. However, the heat associated with their initial and long cycling remains understudied, despite being crucial for a proper understanding of the cell performances. In this study, we utilize optical calorimetry that demonstrates remarkable versatility by providing insights into thermal behaviors at both the cell and material scales. First, we reveal the role of different electrolyte additives on the thermal events occurring during the formation of the solid-electrolyte interphase (SEI) and the cathode-electrolyte interphase (CEI). Sensing proved that the combination of succinonitrile (SN) and prop-1-ene-1,3-sultone (PES) additives significantly mitigates the gas generation during formation for both types of cells, offering a promising pathway to extend 18650 cell lifespan. Next, we study post-formation thermal behaviors through an in-depth entropy analysis, which demonstrates that the higher heat emissions of O3/HC cell compared to P2/HC cell during rate capability tests correlate with the significant irreversibility in the phase transitions of O3 material. In contrast, the P2 phase material shows outstanding structural stability resulting in moderate heat emission, being beneficial for the cell safety. This finding highlights the promising performances of P2 compared to O3 phase cathode material. This work emphasizes the importance of thermodynamic studies in the battery design and highlights the effectiveness of sensing to perform such studies in commercial-type cell.

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*Speaker

Optoelectronics of single and twisted layers of MoS2

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Since the discovery of graphene, two-dimensional materials have attracted significant attention due to their potential applications in next-generation optoelectronic devices.More importantly, the single atomic layer crystal provides an ideal platform to explore fundamental physical mechanisms of electronic transport and electron-photon interactions.
We have divided this project into two parts:

Part 1: Single-layer MoS
Single-layer MoS exhibits a direct bandgap and strong photoresponse in visible light. The electron-photon interaction in this material generates phenomena such as photocurrent and photoluminescence. We systematically investigate the underlying physical mechanisms governing these behaviors under various conditions, including temperature, carrier density, laser power, substrate properties, crystal defects, and environmental adsorbates. The theoretical model developed from this study will help pave the way for future applications of MoS in optoelectronic devices.
Part 2: Twisted-layer MoS
Both experimental and theoretical studies have demonstrated that artificially twisting MoS layers unlocks numerous possibilities for modulating and tuning its optical and electronic properties. At specific twist angles, calculations predict the flattening of valence and conduction bands, resulting in a sharp increase in the density of states and enhanced correlation effects. We aim to explore new phenomena arising from the presence of a moiré superlattice, with a particular focus on unconventional superconductivity it may induce.

Keywords: MoS2, Optoelectronics, Moire superlattice

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*Speaker
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ATP/collagen coacervates as new precursors for bioprinted dense collagen matrices

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Type I collagen received a lot of attention following its prevalence in the ECM of the connective tissue where it provides mechanical support and biological cues for tissue organization. *In vitro*, it presents a hierarchical organization where triple helices assemble into highly ordered collagen fibrils in a process called fibrillogenesis. Combining this bottom-down ability to self-assemble with a top-down technique such as bioprinting is an ideal strategy to mimic the native tissue architecture. However, research on 3D printing collagen is restricted by its use at sub-physiological concentrations making it almost impossible to 3D print collagen solutions in the concentration range required for tissue modeling.

Here, we report a strategy for formulating highly concentrated collagen bioinks with reduced viscosity by using ATP, to change collagen's organisation in a stacked and aligned packing in the form of Segment Long Spacing. This supramolecular arrangement results in a suspension of concentrated coacervates suspended in a solution virtually depleted of collagen. To evaluate the applicability of the coacervates bioink for *in vitro* tissue modeling, its properties were analyzed and compared with collagen in solution in the same concentration range. Rheological tests were conducted showing a ten-fold decrease in viscosity, suggesting an excellent printability in terms of uniform extrusion and preventing nozzle clogging. Microscopic analysis was used to investigate collagen distribution, organization and orientation from molecular to a supramolecular level in fibrillated constructs printed using the new formulation. Moreover, the biological compatibility of this bioink was correlated to the viability, proliferative status and morphology of NHDF in a dense collagen matrix during 14 days of culture.

The inability to bioprint highly concentrated collagen solutions restricts the design of physiologically relevant structures. We show that by changing the molecular organization of collagen molecules into SLS, we obtain a low viscosity suspension compatible with the 3D bioprinting process.

Keywords: Type I collagen, 3D bioprinting, Segment Long Spacing, Coacervation

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[*] Speaker

TiO2-based aqueous battery: how HER contributes to battery death

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Although the current market is dominated by Li-ion technology, aqueous batteries remain widely studied in the hope of addressing issues related to organic electrolytes. While promising, the aqueous approach brings new challenges, the most significant being water electrolysis. Indeed, the insertion/adsorption reactions are limited by the **hydrogen evolution reaction** (**HER**), which constrains the electrode's capacity and stability. Furthermore, **insertion reactions can alter the material** in terms of crystalline structure, electronic properties, and proton adsorption capacity. These changes may enhance **the catalytic activity for HER**. The objective is therefore to study the **water/electrode interface to determine the impact of cation insertion on the electrode's HER activity and its stability**. This information will be valuable in the field of batteries, to better understand how to inhibit HER, as well as in the field of electrolyzers, to explore new catalytic pathways for HER without noble metals. This fundamental work focuses on nanosized anatase TiO2 electrode, originally studied as a negative electrode candidate in aqueous batteries. The goal of this study is to understand what is the potential role played by the inserted cation(s) (Li+, Na+, H+, Mg2+) in TiO2 on the HER thermodynamics and/or kinetics. Ultimately, we intend to use **Operando Electrochemical Spectroscopic Ellipsometry** (OESE) to precisely study the evolution of the optical properties of titanium and thereby monitoring the insertion reactions; while the quantity of each specific inserted cations will be provided by **Operando Electrochemical Quartz Microbalance** (EQCM).

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[*] Speaker

Color in Neo-Impressionism painting: a comprehensive chemical and optical study

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Among the paintings of the 19th century, those of the Neo-impressionist movement (1884-1935) catch the visitor's eye. They are characterized not only by the brightness and luminosity of their colors, but above all by the way they are painted: the canvas is covered with dots of paint arranged side by side, according to scientific theories of color, such as those of M. E. Chevreul, O. Rood and C. Henry (1). At the heart of these rules, optical mixing and simultaneous contrast of color, are mentioned in the manifesto of P. Signac (2). As a result, critics of the time accused them of subordinating art to science.

Ironically, science is nowadays at the service of art: in this thesis, several of P. Signac's paintings were subjected to non-invasive material and colorimetric analyses in order to characterize his palette and better understand his creative process. These studies, combining historical writings with a collection of letters and notes written by P. Signac himself, and an analysis of the color plates associated with these theories, should ultimately shed light on the influence of each of these three color theories on several of his works over the course of his career.

A special attention was paid to his masterpiece *"Au temps d'harmonie"* (1895, Montreuil Town Hall, France). This monumental painting (3 m x 4 m), difficult to access, required the adaptation of the hyperspectral imaging acquisition scheme. The material and colorimetric analyses of this painting faced a major challenge in term of 1) data reduction (3) and 2) data treatment with the use of unsupervised clustering (Fuzzy C-Means and Gaussian Mixture Models). This methodology allowed the identification of P. Signac's palette and provided a deeper understanding of the influence of the three reference color spaces on his painting style.

Keywords: Hyperspectral imaging in the visible range, material and colorimetric analyses, neo, impressionist painting

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*Speaker

Frozen capillary ripples in dried films of polymer solutions resulting from a capillary rise

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When a solid surface is inserted in a thin liquid film, the flow resulting from the capillary rise on the surface is associated with a capillary ripple that propagates away from the meniscus. This effect has been recently evidenced and can be described by the thin-film equation obtained in the lubrication approximation (1). We experimentally study the coupling of this effect with drying in thin films of solutions.

We use polymer solutions with a volatile solvent. Films are spread on a glass substrate, and a glass sphere is placed at the surface of the film at the beginning of drying. First, we observe that the finale dry deposit presents a frozen capillary ripple and a more pronounced ripple closer to the bead (Figure 1.a). We show that the position of the minimum *r_min* is increasing with time, according to a power law in *t^1/4*. Then, in later stage of drying, it plateaus at a final position *r_f* (Figure 1.b). We show that this final position of the minimum of the ripple *r_f* follows a scaling law with the initial film thickness, while a time scale corresponding to the drying time is introduced, i.e., the ratio of the initial thickness of the film and the evaporation rate (Figure 1.c). Futhermore, we observe the formation of another ripple in the meniscus, later in drying, with a different dynamic that the previous one. When a drop of solution is applied and then dried, a crater-like deposit is seen, characteristic of a coffee stain effect (2). We therefore conclude that the final deposit is due to a capillary ripple and a coffee stain in the meniscus. Our results in particular shed light on the industrial problem of dust-induced thickness gradients in dried coatings.

Keywords: polymer — drying — capillary ripple —coffee stain effect

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*Speaker

From Synthesis to Solar Cells: Exploring Lead-free NIR-Absorbing Colloidal Quantum Dots

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The growing demand for clean and renewable energy has driven extensive research into solar cells as a sustainable power source. Among the many types of photovoltaic technologies, quantum dot solar cells (QDSCs) have attracted significant attention due to their unique properties, such as tunable bandgaps, low-cost fabrication, and the potential for high power conversion efficiencies.

Silver bismuth sulfide (AgBiS) quantum dots have emerged as a lead-free alternative with lower toxicity and comparable optoelectronic properties, offering potential for environmentally friendly solar energy applications. Despite this potential, AgBiS QDSCs face two significant challenges. First, the diffusion length of charge carriers is too short, leading to excessive charge recombination and consequently low photocurrent. One approach to address this is the use of plasmonic nanocrystals to enhance light absorption, improving device performance. Second, the traditional synthesis method of AgBiS QDs involves the use of toxic and malodorous trimethylsilyl compounds (TMS), which poses environmental and safety concerns. Therefore, alternative synthesis routes are being explored to mitigate these issues.

Additionally, during the storage of AgBiS-based solar cells in dry air, certain stability-related observations were made, which could contribute to future improvements in the long-term durability of these devices. Further research is needed to optimize both device performance and synthesis methods, while enhancing stability under practical conditions.

Keywords: Quantum dot solar cells, AgBiS, Lead, free photovoltaics, Plasmonic nanocrystals, Solar cell stability, Photocurrent enhancement

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Unforeseen Catalytic Reactivity of Nitrostyrene Derivatives via Supramolecular Catalysis

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Non-covalent interactions have emerged as pivotal tools in the design of ligands for diverse asymmetric catalytic systems. Our group is particularly interested on benzene-1,3,5-tricarboxamides (BTAs)1, disk-like molecules featuring hydrogen bonding groups, which self-assemble into stable threefold hydrogen-bonded helices. Thanks to efficient chirality induction and amplification processes2, BTAs appended with intrinsically achiral phosphine copper complexes demonstrated good efficacy in asymmetric catalysis, providing good enantioselectivities for well-established hydrosilylation and hydroamination reactions3,4. Leveraging this supramolecular catalytic copper hydride system, we probed the reactivity of nitrostyrene derivatives. While 3-nitrostyrene (3NS) followed the classical expected hydroamination pathway, 2- and 4-nitrostyrene (2NS, 4NS) derivatives underwent an unexpected diastereo- and enantioselective dimerization reaction leading to 1,2-diaryl- 1,2-dimethyl ethane derivatives in excellent yields and enantioselectivities (Figure 1). Furthermore, our investigation highlights higher chemo, diastereo and enantioselectivity with supramolecular helical catalysts relatively to conventional ligands. This underscores the distinct advantages of supramolecular catalysis in facilitating unconventional reactivity pathways.

Keywords: Supramolecular polymers, Catalysis, enantioselectivity

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*Speaker

Synthesis of efficient ZnO supported Pd-based nanocatalysts via gas-phase routs

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The central topic of research throughout my doctoral thesis is heterogeneous catalysis. Different, innovative methods are explored for obtaining oxide supported transition metal nanoparticles. The synthesis pathways are centered around gas-phase based methods. All of the catalysts are characterized by various instrumental techniques, leading to better understanding of the composition, crystal structure, morphology and surface properties. Finally, chemical characterization is done by applying the obtained catalysts in environmentally friendly or industrially important reactions. Up until now, the main focus was on Pd-based catalysts supported on ZnO nanopowders. Monometallic Pd/ZnO, was obtained by synthesizing ZnO in the gas phase, followed by liquid phase chemical deposition of Pd-nanoparticles.1 Besides good activity, the catalyst exhibited great reusability potential. One batch of the catalyst was consecutively utilized in three diverse chemical reactions, giving high product yields. Bimetallic PdZn/ZnO catalyst, was synthesized through a one-step gas phase procedure, and was utilized in chemical transformations without any post-synthesis treatments.2 The end goal of the thesis is to correlate differences in catalytic activity with the variations of material properties, occurring as a consequence of differing synthesis pathways.

1. A. Kokanović, V. Ajdačić, N. T. Jovanović, S. Stankic, I. M. Opsenica, *ACS Appl. Nano Mater.* **2023**, *6*, 15820–15828.
2. A. Kokanović, D. Pupavac, S. Chenot, S. Guilet, I. M. Opsenica, S. Stankic, *Catal. Sci. Technol.* **2024**, Advance Article.

Keywords: Nanocatalysts, gas, phase synthesis, Pd/ZnO, PdZn/ZnO

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*Speaker

Tuning Supramolecular Units and Block Copolymers Organization within Polymer Matrices through Macromolecule Functionalization

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Supramolecular self-assembly represents an efficient approach to introduce highly ordered structures in soft matter systems and devices, thereby giving rise to new ranges of properties and functionalities. These structures are formed through the local and dynamic organization of building blocks as a result of non-covalent interactions. Demanding applications can benefit from the combination of several of these forces, particularly for inducing hierarchically ordered structures across a range of length scales. However, targeting the control of hierarchical order on larger length scale through the increase of molecular and supramolecular complexity of a system leads to greater difficulty in structure prediction and higher sensitivity to variations of the method of preparation. It is therefore essential to focus on acquiring a comprehensive understanding of the multi-scale interactions occurring between the various components of ordered systems. In this context, we have explored the hierarchical assembly of block copolymers and small molecular units in a polypropylene matrix. A series of increasingly complex compositions were targeted, ranging from a simple blend of PS and PP to a blend of these polymers compatibilized with a polystyrene-block-poly(ethylethylene)-block-polystyrene block copolymer bearing pendant supramolecular motifs. These materials were prepared in the melt by extrusion, and they were studied using a comprehensive set of analytical techniques, probing the system at multiple length scales. We have uncovered intriguing non-orthogonal assembly behavior between the supramolecular polymer, the unfunctionalized block copolymer, and grafted derivatives of the block copolymer, giving rise to striking consequences to the structure of the final materials.

Keywords: Supramolecular chemistry, Material science, Self assembly, Hierarchical structures

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Self-assembled hydrogels from bio-based amphiphiles

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Bio-based amphiphiles, developed as sustainable alternatives to petrochemical surfactants, are highly attractive amphiphilic compounds due to their stimuli-driven self-assembly properties. Among a wide range of potential applications, their use in cosmetics and personal-care products, requires the study of their viscoelastic properties, yet their potential as gelators has only recently begun to be explored. In this work, two bio-based amphiphiles, a glycolipid, GC18:1 and a lipopeptide, surfactin are shown to form hydrogels in response to different stimuli, upon the introduction of metal ions or pH reduction, respectively. To enhance the performance of such gels and broaden their application scope, efforts have been made to better control their mechanical properties and to integrate inorganic nanostructures into the hydrogels. Incorporation of dynamic cross-linkers and coupling the sugar groups of the glycolipids with boronic acid, led to changes in the rheological profile of the gels, although further investigation is required to fully understand the mechanism involved. Additionally, the integration of metal nanostructures is achieved by in situ reduction of a silver-coordinated glycolipid gel, resulting in anisotropically aligned silver nanoparticles of controlled size, which coalesce into silver nanowires with electron-conductive properties. The gels are characterized by a wide range of methods including small angle X-ray scattering (SAXS), cryogenic transmission electron microscopy (Cryo-TEM), rheology and impedance spectroscopy.

Keywords: bio, based amphiphiles, hydrogels, self, assembly

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*Speaker

Exploring transformations in elemental sulfur using a machine-learned interatomic potentia

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We investigate liquid polymorphism in elemental Sulfur, using atomic-scale simulations in the form of molecular dynamics, with a focus on both the lambda- and the liquid-liquid transitions. We propose a DFT-ML workflow that is general enough to study liquid polymorphism, which aims to produce a machine-learned interatomic potential (MLIP) to explore phase diagram regions efficiently.

Our workflow employs various MLIP architectures, based on the complexity of the task at hand, alongside active learning protocols. For instance, we use efficient models in the form of Behler-Parrinello neural networks for structure selection through "query by committee" and equivariant MLIPs for the final regression task. To enhance the stability, accuracy, and overall generalization capability of the final MLIP, we addressed multiple aspects: managing van der Waals interactions analytically, evaluating potential energies and forces on the training dataset using hybrid DFT, and implementing a recursive training approach.

With our model in hand, we are able to reach system sizes and timescales unattainable at the DFT level. We explore specific zones of the phase diagram in the surroundings of the transition lines using unbiased molecular dynamics, as well as simulations involving enhanced sampling along specific collective variables.

Concerning the liquid-liquid transition, we compare our findings with experimental data and results obtained at the DFT-LDA level of theory.

Keywords: MLIP, transitions, liquids

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*Speaker

Reducible Fe-MOFs for the environmental abatement of NOx

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Air pollution is an important issue, particularly in urban areas, and is linked to combustion processes. The emission of nitrogen oxides (NOx) constitutes a critical environmental problem, and it can affect severely human health. The main two components are nitrogen monoxide (NO) and nitrogen dioxide (NO2) and come from different human sources. The first source of emission comes from the motor vehicles, especially diesel engines, due to high-temperature combustion. Burning fossil fuels in power plants to generate electricity also releases significant amounts of NOx as well as industrial processes, such as nitric acid production and fertilizer manufacturing. It can cause smog and respiratory problems such as asthma and increase the risk of cardiovascular and respiratory diseases1. The World Health Organisation has updated its recommendations on exposure to nitrogen oxides for 2021: Annual average concentration of nitrogen dioxide (NO2): 10 μg/m3 compared with 40 μg/m3 according to the 2005 guideline. The current catalytic degradation technique is SCR (selective catalytic reduction) which requires both high temperature conditions (300-400$\circ$C), a catalyst who plays an important role (V2O5-WO3/TiO2) as well as sacrificial agent (ammonia or urea) to transform the NOx into harmless gases (nitrogen and water). This leads to an efficiency of over 90% under the right operating conditions2. Metals-Organic-Frameworks (MOFs) are crystalline porous materials that can be a good alternative to the current SCR catalyst. In particular, the mesoporous iron trimers based MOF denoted MIL-100(Fe) (MIL stands for Materials from Institut Lavoisier), once carefully thermally reduced into a mixed valence Fe(III/II) material, has demonstrated at room temperature, in the presence of oxygen and humidity, without the need of a sacrificial agent, an unprecedented conversion of NOx into N2 and O2.

Keywords: Matériaux poreux, catalyse, NOx

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*Speaker

Cyclable and cheap catalysts for hydrogen storage and release by organic liquids

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Hydrogen use is a promising solution for the development of a low-carbon economy but several technical locks still remain and prevent its efficient use, including in H2 storage and transportation.(1) One of the most appealing solution to this problem is the use of Liquid Organic Hydrogen Carriers (LOHC), organic compounds that can absorb and release a high weight fraction of hydrogen through chemical reactions.(2) Their usage makes possible the storage of H2 under ambient conditions, avoiding the problems linked with storage under high pressure as well as its flammability.

The aim of this thesis is therefore the development of new, affordable, energy-efficient and cyclable catalysts based on metallic nanoparticles immobilised on different supports for the hydrogenation and dehydrogenation of primary amine/nitrile pairs (LOHC). The first step of the project is the synthesis of a library of Co, Ni, and CoNi colloidal nanoparticles of various shapes and sizes, then their immobilisation on different supports such as porous silica particles, Si-wafers, or carbon nanotubes. Finally, the activity, stability and cyclability of the catalysts (colloidal and supported) for the hydrogenation of nitriles and dehydrogenation of amines will be studied to characterise the effects of the morphology of the nanoparticles and the type of support.

1. Schwaab, V. *et al.* Liquid Organic Hydrogen Carriers: Model Catalytic Studies on the Thermal Dehydrogenation of 1-Cyclohexylethanol on Pt(111). *J. Phys. Chem. C* 127, 11058–11066 (2023).
2. He, T., Pei, Q. & Chen, P. Liquid organic hydrogen carriers. *J. Energy Chem.* 24, 587–594 (2015).

Keywords: nanoparticles, nanoalloys, chemical storage of H2, heterogeneous catalysis

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[*] Speaker

Oxythiohphosphates ionic conductors for all solid-states batteries

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Solid electrolytes (SEs) have attracted significant attention for developing all-solid-state batteries (ASSBs), which could enable the use of Li metal as the anode, thus improving both energy density ($>$ 1500 Wh/L) and safety (1). Intensive research has focused on developing new materials as SEs, leading to the discovery of the lithium superionic conductor Li10GeP2S12 (LGPS) with higher ionic conductivity ($>$ 10-2 S cm-1) compared to the liquid ones (2). However, LGPS has issues with electrochemical and chemical stabilities preventing its use in ASSBs. To overcome these issues, sulfur was partially substituted by O, forming Li3PS4-xOx (where, x$<$ 1) compositions with LGPS like-structure, and exhibiting improved electrochemical chemical stabilities. High-temperature synthetic pathways, however, result in a complex mixture of different anions (PO43-, PO3S3-, PO2S23-, POS33-, PS43-) at the local scale, without precise control on their proportions and distribution. This limits the range of possible compositions in the Li-P-S-O phase diagram. The goal of our research is to explore the Li-P-S-O system using a low-temperature approach to achieve better control of the stoichiometry and repartition of anions. We seek to extend S substitution by O across the entire composition range by obtaining all pure lithium oxythiophosphates: Li3PO3S, Li3PO2S2, and Li3POS3. Currently, there is no studies in the literature that have reported or discussed the Li-P-S-O system via wet chemistry. Our work takes inspiration from the Na-P-S-O system, in which the Na3PO3S, Na3PO2S2, and Na3POS3 phases were successfully stabilized as pure compounds in water at low temperatures (3).

(1) Albertus, P. et al., ACS Energy Lett. 2021, 6, 1399–1404.

(2) Kamaya, N. et al., Nat. Mater. 2011, 10 (9), 682–686.

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Keywords: Ionic conductors, All solid, state batteries, Oxytiophosphate

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[*] Speaker

Superconductivity in strongly overdoped cuprate

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Recent reports show that some cuprates, such as Cu0.75Mo0.25, Sr2YCu2O7+x and Ba2CuO3+x, exhibit high-Tc superconductivity in the 80-90 K range in the strongly overdoped regime, for doping levels p_˜0.4 hole/Cu or higher, well beyond the superconducting dome, where a conventional Fermi liquid behaviour is rather expected. This surprising result, achieved by means of high-pressure oxygenation, raises the question of whether the holes provided by the extra oxygens, x, contribute to the superfluid density or rather form a phase-separated metallic phase. In order to address this point, I investigate the average and local structures of a series of YBa2Cu3O7+x/ HgBa2CuO4+x samples with different oxygen concentrations up to x=0.4 or larger, by means of X-ray, Raman, SEM-EDX, SQUID measurement and Heat capacity, corroborated by synchrotron diffraction data refinement. I engaged to determine the local order of the extra oxygens, which shall enable to establish a correlation between x, electronic structure, and normal-state and superconducting properties.

Keywords: Superconductivity, Cuprate, Overdope, High Pressure Oxygen Synthesis

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*Speaker

Optimal reaction coordinates from the projected dynamics of transition paths

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While generic collective variables (CV) indicating the progress of a transformation are ubiquitously used to model physico-chemical processes, finding optimal reaction coordinates (RC) that yield accurate thermodynamic and kinetic properties is a fundamental challenge in the field of atomistic simulations. The aim of this work is to provide a rigorous and computationally affordable method to optimize RCs. In fact, the dynamics of a system projected on a CV can be modeled through Langevin equations. Recently, our group showed that accurate free energies and rates can be extracted from transition path sampling trajectories by optimizing overdamped Langevin models via likelihood maximization. However, the quality of the CV defines how accurately the Langevin model can reproduce the original dynamics. We proposed an inexpensive method to optimize RCs in post-processing analysis. The approach is based on a variational principle stating that low-dimensional stochastic models of high-dimensional dynamics yield kinetic rates larger or equal to the original one: minimizing the kinetic rate of the effective dynamics predicted by Langevin models – as a function of the CV employed – yields the optimal RC.

Using as input a set of short, unbiased molecular dynamics trajectories from aimless-shooting transition path sampling, we define a putative CV as a combination of simple, physically based CVs, and we optimize parameters of such combination minimizing the rate of the corresponding model. After tests on a benchmark analytical system, we apply the method on two complex processes: the interaction of fullerene dimers in water, as well as the association/dissociation of a protein complex in water. Our results indicate that it

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*Speaker

is feasible to simultaneously estimate free-energy landscapes, kinetic rates and optimal RCs on complex systems at moderate computational cost.

Keywords: Computational physics, biophysics, rare events

Constant voltage breakdown measurement of lapped insulation under cryogenic conditions

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• The SCARLET project innovates superconducting cables to connect remote renewable energy sites to the grid, focusing on high-temperature superconducting (HTS) and low-temperature superconducting (MgB_2) cables
• A cryostat with a moving electrode is used to test cylindrical lapped insulation samples, simulating actual cable manufacturing conditions and providing consistent environmental testing
• The results demonstrate that these cylindrical samples yield more accurate voltage breakdown measurements, closely reflecting the real behavior of superconducting cables compared to traditional flat electrode methods

Keywords: Superconducting, hydrogen, insulation

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Unravelling the roles of texture and basal lamina composition on the endothelialization of biomimetic type I collagen matrices

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Understanding cell-surface interactions on the luminal surface of arteries is key for vascular grafts' development. In vivo, the basal lamina (BL) lines the luminal surface of arteries and is mainly composed of two collagen IV and laminin networks. It provides biological and mechanical cues favoring endothelial cells' adhesion, proliferation, and activity, essential for blood vessels' integrity. Beyond composition, the nanometer or micrometer scale topography of BL also regulates cell morphology and activity. However, the effect of composition and topography on endothelialization remains entangled and little tools are available to decorrelate their effects. Here, highly concentrated macroporous type I collagen constructs mimicking the extracellular matrix of blood vessels were produced through ice templating followed by topotactic fibrillogenesis. We used this new biomimetic model of the arterial wall extracellular matrix to evaluate the combined effect of composition and topography on the surface of biomimetic substrates (6). Thus, we have fabricated materials that feature different topographies on each side: a smooth surface and a textured one with ridges and grooves. Each of these surfaces was coated with BL proteins: laminin, fibronectin, or collagen IV. Surfaces were characterized by scanning electron microscopy and confocal microscopy. To investigate cell-surface interactions, materials seeded with bovine aortic endothelial cells were observed with fluorescent and confocal microscopy. We observe endothelial cells' adhesion on the surfaces, and their higher ability to produce VE-Cadherin and therefore form a tight monolayer on a smooth surface. Besides, we notice that unidirectional micrometer scale patterns induce a preferential orientation of the cells. Quantitative results on cell density, metabolic activity and proliferation enable for the first time to decorrelate the role of topography and composition on biomimetic substrates. The results open an exciting pathway to enhance endothelialization of biomimetic materials for vascular tissue engineering and better control colonization kinetics regulated by topography.

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*Speaker

Keywords: arterial wall model, basal lamina, endothelialization

Shaping the Photoluminescence of Infrared-Emitting Mercury Telluride Nanocrystals Through Their Coupling to Photonic Structures

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Infrared-active colloidal quantum dots (CQDs) have recently emerged as a powerful alternative to traditional epitaxially grown semiconductors, in part for light emission purposes. Notably, Mercury Telluride (HgTe) CQDs show bright photoluminescence and electroluminescence which can cover a wide range of wavelengths (1-5 μm), corresponding to a breadth of practical applications (active imaging, spectroscopy, LIDAR, ...). While in the visible the use of CQDs as light emitters has reached commercial levels of development, further efforts are still needed in the infrared. Indeed, HgTe CQDs suffer from a strong drop in efficiency after device integration, going from up to 75% in solution to 0.5% on average once inside light-emitting diodes (LEDs). To remedy this issue, a key component is the efficient extraction of light from devices. In most LED structures, only 20% of generated photons radiate to the outside, due to internal reflections and waveguiding at the different material interfaces. A possible strategy to solve this problem is to couple the CQDs' emission to a photonic structure. This enables control over light-matter interactions and the possibility to design the electromagnetic field's shape inside the LED. When properly designed, these structures can grant directionality to an isotropic emission and in theory ensure the outcoupling of most photons in light-emitting devices.

To demonstrate this strategy, we integrated HgTe CQDs to different photonic structures compatible with future device functionalization, from plasmonic metallic gratings to full-dielectric cavities, through simple solution processing techniques. The resulting coupling led to enhanced luminescence properties from the CQDs, such as a 2-fold increased photoluminescence magnitude, a strong directivity down to 15◦ around normal incidence, and a decreased spectral linewidth by a factor of 10. These results advance the realization of optimized and efficient HgTe-based LEDs in the infrared.

Keywords: Infrared, Nanocrystals, Photonic structures, Photoluminescence

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[*] Speaker

Soft biomaterials associating microfibrillar collagen I with nanostructured chitosan

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Type I collagen and chitosan are two of the most studied and used biopolymers for hydrogel manufacturing. Although several mixed materials have already been reported, their combination within dense physical networks remains challenging due to high viscosity as well as rapid phase separation occurring when using concentrated starting solutions. In this work, we disclose an efficient protocol based on highly concentrated acidic solutions of both biomacromolecules to form homogeneous hydrogels, containing up to 30% (w/w) collagen I, with controlled micro- and nanostructures. Multiscale characterization highlights that the mixed network organization, from composite to hybrid structures, is dependent on the gelation route. In particular, unusual collagen I branched fibrillar structures can be observed within a nanostructured chitosan network. The difference in the kinetics of self-assembly/gelation between the polymers appears to be a key parameter driving mixed network organization. The gelation route also influences rheological and mechanical properties of the hydrogels, in particular the impact of collagen I on the chitosan network stability. Accordingly, the ability of collagen to promote metabolic activity and proliferation of normal human dermal fibroblasts in vitro depends on both its content and the gelation route.

Keywords: Hydrogel, Collagen, Chitosan

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*Speaker

CVD/MBE hybrid rare earth oxide thin films for on-chip quantum technologies

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Oxide crystals doped with rare-earth ions (such as Eu:Y2SiO5) are promising materials for quantum technologies. This is due in particular to their long **coherence time**, corresponding to the period during which it is possible to maintain or manipulate a quantum state. On the other hand, in a context of device miniaturization and to exploit enhanced light-matter interactions, nanomaterials such as **thin films** and nanoparticles are advantageous alternatives to the use of bulk crystals. However, some material properties are strongly affected by miniaturization and in particular coherence time. The aim of this work is to solve this problem by optimizing the fabrication process, so that films with good coherence properties can be produced industrially. To this end, the deposition technique used to create our oxide films is **DLI-CVD** (Direct Liquid Injection chemical vapor deposition), which is commonly used in the electronics industry. As coherence is strongly affected by the environment, the strategy is to minimize defects by making **epitaxial films** (Fig.1 a) and c)). These crystalline films are oriented with respect to the substrate, unlike polycrystalline films that consist of randomly oriented grains (Fig.1 b) and d)). It is thus expected that better coherence properties could be achieved with the more ordered epitaxial films.

In this project, we have successfully grown polycrystalline films and even epitaxial films by changing the substrate type. SEM images, XRD measurements and optical measurements: photoluminescence spectra, decays and inhomogeneous linewidth measurements; prove the good quality of all films. After selecting the most promising substrates, we improved the optical properties of the films by applying different annealing treatments.
In the future, we plan to continue the improvement of the post-treatment conditions of the films as well as to develop nanostructuration by lithography and etching, a necessary step towards their integration into the desired resonators or waveguides.

Keywords: CVD, thin films, quantum technologies

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[*] Speaker

Silica-coated Gold Nanorods for controlled release of genetic material under NIR laser light irradiation

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Gold nanorods (AuNRs) are anisotropic nanoparticles displaying interesting optical properties, which make them candidates of choice for biosensing, drug delivery and photothermal therapy. Their shape induces two localised surface plasmon resonance (LSPR) bands, along the transverse and longitudinal axes of the gold nanobead.(1,2) In the case of AuNRs, the position of the longitudinal LSPR band can be finely tuned from 600 to 1800 nm by controlling their aspect ratio. (3) Their synthesis requires the use of cetyltrimethylammonium bromide (CTAB), which acts as a surface stabiliser and shape-inducing agent. However, in addition to complicating the chemical functionalisation of AuNRs, CTAB is known to be cytotoxic, thus limiting the use of AuNRs for biomedical applications. Covering the AuNRs with a layer of silica increases their biocompatibility and provides an interesting functionalization surface for biomolecules grafting.(4)
In addition, the silica shell stabilises the anisotropic nanoparticles under irradiation, making these 'core-shell' systems great candidates for photothermal therapy or irradiation-induced delivery of genetic material.(5)

In this work, the coating of AuNRs with a silica layer is explored by varying several parameters such as pH of synthesis, reagents ratios as well as reaction time in order to control silica thickness and porosity. The formed core-shells are then extensively characterised by UV-Visible spectroscopy, HR-TEM, DLS, ξ potential and XPS. The optimal conditions for AuNRs coating with a homogeneous silica shell of controlled porosity and thickness are discussed, while preserving the AuNRs optical properties.These core-shell nano-objects are then used to graft

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oligonucleotide duplexes and release them under laser irradiation.

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PROTON CONDUCTIVE MOF-BASED MIXED MATRIX MEMBRANES FOR FUEL CELL APPLICATIONS

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Proton Exchange Membrane Fuel Cells (PEMFCs) show great potential as clean energy solutions, converting hydrogen into electricity efficiently. However, their widespread adoption is hindered by limitations in current membrane materials. Nafion, the leading proton exchange membrane, faces several challenges, including high costs, gas leakage, environmental concerns during production, an unclear proton conduction mechanism, and dependence on high relative humidity and temperature.1 Metal-organic frameworks (MOFs) have emerged as promising alternatives due to their customizable structures, large surface areas, and excellent proton conductivity.2 Nevertheless, the powder nature of MOFs necessitates integration into a polymer matrix, forming Mixed-Matrix Membranes (MMMs). By combining MOFs' advantages with polymers' mechanical strength, flexibility, and gas control, MMMs offer a compelling pathway to next-generation, high-performance PEMFCs.3

Water-stable nano-MOFs, renowned for their high proton conductivity, were synthesized using environmentally friendly and scalable methods.4–6 These MOFs were subsequently integrated into bio-sourced and water-soluble polymers such as polyvinyl alcohol, chitosan, and carboxymethylcellulose. A comprehensive study explored the influence of MOF content, MOF-polymer interactions, and polymer composition on the resulting MMMs. The structural properties of these membranes were characterized through X-ray diffraction (XRD), dynamic scanning calorimetry (DSC), thermogravimetric analysis (TGA), scanning electron microscopy (SEM), and other techniques. Proton conductivity was measured via electrochemical impedance spectroscopy (EIS).

Stable and smooth MOF/polymer composite membranes were developed by optimizing nanoparticle MOFs to prevent aggregation and maintain membrane quality. Key factors, including filler ratio, casting thickness, and polymer concentration, were also fine-tuned. These eco-friendly MMMs exhibited superior proton conductivity compared to pure polymer membranes, highlighting the synergistic interaction between MOF and polymer. This improvement is likely due to a favorable interfacial structure that enhances proton mobility. These results demonstrate the immense potential of biodegradable MOF-based MMMs as advanced PEMs, offering a promising solution to traditional PEM challenges for more sustainable, efficient fuel cell systems.

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Keywords: MOFs, Mixed Matrix Membrane, Proton Exchange Membrane, Fuel Cells

Thermal stability of High Entropy Alloy Nanoparticles: an atomic scale study

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High-entropy alloy nanoparticles (HEA-NPs) have recently been synthesized and shown promising catalytic properties. To explore their potential in medium or high temperature application beyond catalysis,it is crucial to understand their thermal behavior and structural stability. In this study, we combined Molecular Dynamics (MD) simulation with *in situ* aberration-corrected Scanning Transmission Electron Microscopy (STEM) observations to gain atomic-level fundamental insights into the thermal stability of CoNiCuPtAu HEA-NPS. Experimentally, in situ STEM was used to study the evolution of the structure and composition of CoNiCuPtAu HEA-NPsfrom 300 to 973K, in real time and on an atomic scale.The stability of the NPs was demonstrated up to a temperature of around 773K, where a segregation of gold and copper on the surface was observed within coalesced NPs.Above 973K, a significant loss of gold and copper was observed on all NPs.

To gain fundamental insights into the atomic and kinetic/thermodynamic origin of the temperature-driven structure transition observed experimentally, we performed MD simulation, using the LAMMPS code based on the Zou et al potential, to investigate the structure of CoNiCuPtAu NPs under thermal stimuli.
In this context, 309 to 3871-atom CoNiCuPtAu HEA-NPs in equiatomic composition were considered. The investigation of their structural properties over the temperature range from 400 to 1500 K, results in a number of significant conclusions. Firstly, in good agreement with experimental observation, a temperature-dependent segregation of gold and copper at the NP surface is highlighted. Furthermore, the analysis of the local atomic energy of the different elemental species confirms the strong tendency of Au and Cu atoms to segregate at the surface. The Au and Cu surface atoms have the lowest energy and are therefore highly susceptible to evaporation, which may explain their depletion in the NPs at high temperature as observed experimentally.

Keywords: Nanoparticles, high entropy alloys (HEA), atomistic simulations, in situ transmission electron microscopy

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*Speaker

Tuning optical properties of acrylate films using self-patterning

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Controlling the optical properties of materials, especially glass is crucial. One of the most desirable properties is the ability to control blur particularly in the production of matte glass. Currently, hydrofluoric acid-based processes are commonly used to achieve this effect but the blurring is often less well-defined and the method is not environmentally friendly. A more sustainable alternative is to apply a polymer coating to these surfaces. Photopolymerization is the most widely used industrial technique for producing thin films. We observed that under specific conditions photopolymerization of low Tg acrylate monomers results in films with well-defined surface morphologies, such as lamellae or hexagonal structures(1). These patterns are due to spontaneous swelling of the film surface by unreacted monomers(2). We demonstrated that the optical properties of these films (such as haze and clarity) are linked to the type and size of the surface morphologies which can be finely tuned by adjusting the UV lamp intensity even with the same formulation. However these soft films exhibit poor mechanical properties. In this study we extended the process to high Tg acrylate monomers by adapting the formulations. We found that the mechanical properties of the films were improved without compromising their optical properties. In particular for tert-butyl acrylate, we discovered a new regular morphology that gives the film an iridescent effect.

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Keywords: photopolymerization, self patterning, coatings

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Catalytic materials for the valorization of CO2 from diluted sources

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The amount of CO2 in the atmosphere has raised up to 0.04% due to anthropogenic emissions, leading to climate change. As the result, there is an urgent need to remove its excess in air and reduce our carbon footprint. Carbon capture at sources, *e.g.* in industrial flue gases (up to 14%1), is the very first step and is ideally combined with its use in chemicals or fuels and its storage (CCUS technology). CO2 uptake requires bases and proceeds either by absorption with amines or adsorption with materials such as earth alkaline oxides, including magnesium oxide. MgO is a versatile and low-cost material but often suffers from low textural properties2. In the present work, an original pathway has been proposed in order to increase significantly the specific surface area of commercial MgO by forming a gel of magnesium carbonate in MeOH under CO2 pressure, drying it after removing the excess of MgO, and treating the recovered Mesoporous Magnesium Carbonate thermally. The MgO obtained (120 cm3.g-1) was deeply characterized and successfully tested as a catalyst for the coupling of C-C bonds under basic conditions (Claisen-Schmidt condensation) as well as for the formation of cyclic carbonate from the cycloaddition of CO2 onto epoxide which is a valuable approach for CO2. Interestingly, the addition of various amounts of Ni(II) salts in the gel formed intermediately allowed, after drying and thermal treatment, to prepare mixed oxides of Ni and Mg with 4.2 wt.% $<$ Ni loadings $<$ 12.8 wt.% in a simple way. After reduction at 900◦C under hydrogen, resulting materials were tested as catalysts for the reduction of CO2 into methane. The highest activity was obtained with the mixed oxide loaded at 8.5wt.% This catalyst was stable for 12 h and led to 70% conversion of CO2 and 98% selectivity of CH4 at 355◦C.

Keywords: high surface magnesium oxide, One pot method, Claisen, Schmidt condensation, CO2 methanation

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Luminescent nanoparticles: from synthesis to nanothermometry for the control and understanding of magneto-induced process

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Temperature is one of the most common physical quantities and significantly contributes to chemical reactivity and biological processes. Nanothermometry by luminescence is related to temperature measurements at nanoscale with high spatial ($< 10\mu$m) and temporal (0.1s) resolution using nanoparticles. The temperature dependence of luminescence can be expressed by the evolution of one or more parameters such as: shift in the emission peak position, band shape, peak broadening, intensity variation, polarization evolution, or lifetime.

Many teams around the world are interested in these nanothermometry challenges, with additional constraints due to the complex systems in which these thermometers are used. To better evaluate these various nanothermometers, relative sensitivity (Sr) has been introduced as a performance criterion. A nanothermometer is considered effective when its relative sensitivity is greater than 1%K-1 over the studied temperature range. This threshold is difficult to achieve and is highly dependent on the materials used. The main problem with this technique is the reliability of the temperature measurement due to the variation of certain optical parameters depending on the concentration of the particles or their environment. Thus, the community agreed on the importance of numerically processing the collected data in order to calculate parameter ratios for more accurate temperature measurement.

To meet the demand for nanothermometry probes, the scientific community tends to focus on lifetime measurements that require expensive equipment, or ratiometric method. This project falls within the latter approach, with the goal of conducting nanothermometry measurements using spinel-type AB2O4 oxide nanoparticles doped with transition metals (luminescent centers). In an effort to enhance sensitivity, we are focusing on small doped nanoparticles ($<$ 20nm) synthesized via a hydrothermal method assisted by microwave heating. The project aims to measure the temperature of magnetic nanoparticles (heating particles) using luminescent nanothermometers in a liquid environment over a range of 50 to 300$\circ$C.

Keywords: Nanothermometry, Nanoparticles, Oxide Materials, Microwave heating

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*Speaker

Study of the knee-point (sudden death) of Li-ion cells by optical sensors

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The onset of the knee point in lithium-ion batteries, marked by a rapid decline in performance, is closely tied to the elusive phenomenon of lithium plating, which remains a key challenge in extending battery life and ensuring safety. In this work, we present a novel approach to understanding the lithium plating mechanism by embedding Fiber Bragg Grating (FBG) sensors within of both custom-built and commercial pouch cells. These sensors provide real-time monitoring of strain, enabling us to capture the intricate "breathing" behavior of the cells as they undergo volumetric expansion and contraction during electrochemical cycling. By linking strain dynamics to both internal electrode behavior and surface deformations, we detect a correlation between the strain signals and the onset of lithium plating, which precedes the knee point. This method links strain with electrode volume expansion and lithium plating, revealing a pathway for early detection of failure. Our findings offer a powerful tool for in situ monitoring, providing new strategies for improving battery longevity and safety.

Keywords: Knee, point, lithium, ion batteries, lithium plating, Fiber Bragg Grating (FBG) sensors

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*Speaker

Ice mixtures (H2O,NH3 and CH4) under extreme pressure and temperature conditions

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Water, ammonia and methane are the major components of the interiors of Neptune and Uranus, as well as several satellites (Titan, Ganymede, ...) and exoplanets. In these natural bodies, these ices would exist under extreme pressure and temperature conditions (up to several Mbar and thousands of K) and the astrophysical observations (magnetic fied, gravitational moment...) would be directly linked to their properties. Unfortunately, the experimental determination of the physical-chemical properties of the icy mixtures under extreme conditions is lacking and moreover, the exact composition of the icy layers is still unknown. Moreover, from a fundamental perspective, these ice mixtures are ideal systems for studying the evolution of hydrogen bonds with density. If unconventional phases have been reported in water/ammonia ices, the influence of methane (which does not form H-bonds at normal conditions) is unknown and remains to be explored. During my thesis, we extended the experimental exploration of the water-ammonia mixtures by studying their phase diagrams at high pressure (0-20 GPa) and high temperature over a wide range of concentrations in diamond anvil cells (DAC). By combining X-ray diffraction and Raman experiments, we were able to build Isothermal binary diagrams up to 700 K and determine all the different phases of the ($H2O$-$NH3$) system as a function of pressure and composition. By coupling all of these binary diagrams, we will obtain a 3D phase diagram (P, T, composition) of the water-ammonia mixtures, which constitutes a crucial database for planetary modeling. Actually, now that we have a better understanding of the ($H2O$-$NH3$) system, we have complexified the mixtures by adding methane. After designing a new protocol to load the ternary ice mixtures in DAC, we have conducted a first XRD synchrotron experiment to explore their HP-HT properties. The analysis of the data is in progress.

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Keywords: high pressure, ices, high temperature, icy planets, hydrogen bonds, phase diagrams

Cavity based photoconductive antennas for coherent detection of THz QCLs

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Photoconductive antennas (PCA) are used in terahertz technology as emitters or detectors. They are typically employed to generate/detect broadband THz pulses covering the frequency range from 0.1 to 4 THz. This device has been widely accepted as a reliable source and detector for THz generation and detection and are useful in many applications, such as time-domain spectroscopy which requires broad spectra sources or multiinput multi-output (MIMO) communication. Nevertheless, this technology presents shortcomings in detecting weak terahertz signals and improving the Signal-over-Noise-Ratio.This is mainly due to a low optical-to-THz conversion efficiency and to the dissipation of THz waves in the semi-conductor substrate. A concept of creating of THz cavity by burying a metal layer has then been studied to enhance THz detection with PCA devices. Photoconductive switches operate on the effect of ultrafast variations of surface photoconductivity of a semiconductor substrate under fs-laser excitation. The devices are usually composed of several electrodes spaced by a certain gap and deposited onto a semiconductor surface. The excitation of the gaps between the electrodes biased by an external voltage creates a sharp increase of concentration careers which generate the THz pulse. However, the recombination of free carriers in standard GaAs substrate is too long to be used in detector devices for time-resolved coherent detection. The solution is here to use LT-GaAs material which present low carrier lifetime due of its important concentration of defects. The sample was build using wafer bonding technique. This antenna showed an important detected spectrum shift and a significant signal-over-noise ratio around 3THz. This shift allowed the detection of first QCL oscillations, the QCL emitting at 2.8THz.

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Macroscopic Access Resistances Hinders the Measurement of Ion-Exchange-Membrane Performances for Electro-Dialysis Processes

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Since the beginning of blue-energy harvesting research, a lot of advances have been made about membrane design and nanofluidic diffusio-osmotic transport, but the efficiency gap of 6 orders of magnitude between nano-scale designs and industrial power plants remains unsolved. Just after synthesis, selective membranes are benchmarked on very small samples on the basis of the output power. This method of power per unit area based on membrane resistance is therefore a key point to compare several devices and their efficiency.
An electrochemical cell has been used to place a selective membrane of varying area between two electrodes. The membrane resistance and power density have been experimentally measured. This systematic study shows that the membrane resistance is inversely proportional to the square root of its area. Whereas it's currently assumed that the resistance and the area of a membrane are inversely proportional. Based on this assumption, the power density is believed to be independent of the membrane area, which we prove to be wrong. This result has a big impact on the reliability of the power density announced in the literature for different devices: the smaller the area of the tested membrane the higher is the output power density: from 0,5 W/m^2 up to 150 W/m^2 for the same membrane, same salt ratio (100) different membrane areas. This leads to overly optimistic extrapolation of electrical performances for membranes engineered and tested at sub millimeter sizes that will be industrially used at meter sizes.
To explain these results, we developpe a model using diffusion equation across a nanochannel. Experimental data and theoretical modeling are corroborating without any adjustment parameters. Consequently, the power per unit area obtained at micro scale cannot be extrapolated a priori to larger membranes. So, the comparison is biased between large scale commercially available membranes, and nano-engineered microscale membranes.

Keywords: Blue energy, nanopores, ion exchange membrane, Electrodialysis

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[*] Speaker

A nonlinear variational model of cracks and dislocations

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In crystalline materials, fracture is often coupled with plastic activity. A comprehensive mesoscale modeling of fracture should therefore incorporate crack propagation and its interplay with dislocation multiplication and glide.
Both cracks and dislocations are associated with discontinuities in the displacement field. Therefore, it should be possible to construct a model based only on the displacement field. This requires the identification of a nonlinear elastic energy functional that is invariant with respect to the point group of the lattice, but also with respect to any shear deformation that leaves the lattice invariant.

In this talk, we show how to construct this infinitely degenerate potential energy and discuss the numerical implementation of the model. Finally, we present simulation results that reproduce spontaneously, through the dynamics of the displacement field alone, the complex interplay between evolving fractures and dislocations, including dislocation nucleation at the crack tip and crack nucleation due to strain localisation generated by dislocation glide.

Keywords: crack, dislocation, variational model, nonlinear elasticity, multi, physics approach

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Topochemical synthesis in molten salts: towards new compounds of transition metals and p-block elements

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Topochemical reactions are post-modifying material compositions with slight changes in their crystal structures. When applied to nano-objects, these approaches enable to reach complex compositions and shapes, but they imply using low temperature colloidal synthesis, which limits their use to ionic or metallic solids. Post modifications of more covalent materials would pave the way to specific properties, related to (electro)catalysis, magnetism, and hardness, for instance, but they require higher temperatures. The aim of my Ph.D. work is to develop topochemical reactions on covalent materials by using liquids to make these reactions feasible at relatively high temperatures, thereby giving access to new compositions. I use molten salts as thermally stable liquids and focus on two families of topochemical reactions: galvanic replacement and cation exchange.

We are investing the galvanic reactivity of Mo-MAX phases (Mo2TiAlC2, Mo2Ti2AlC3 and Mo1.66Y0.33AlC) in oxidative molten salts to synthesize potential 2D nanocatalyst. Indeed, oxidative molten salts enable the exfoliation of lamellar MAX phases: transition metal (M) carbides or nitrides (X), separated by layers of Al, Si, or Ga (A) into MXenes: 2D nanomaterials.(1–3). MXenes synthesized from these Mo-based MAX phases might exhibit interesting electrochemical properties notably for the hydrogen evolution reaction (HER) because Mo atoms would be localized outward the layers and can undergo reversible changes or oxidation states.(4)

In a second hand we are focusing in cation exchange on CuSi2P3, a promising electrocatalyst which reduce carbon monoxide into acetate, with the aim of modulating its (electro)catalytic properties. CuSi2P3 is a iono-covalent structure, which can be described as Cu+(Si2P3)-. We are targeting the isovalent substitution of Cu+ by Ga+ and In+ and aliovalent substitution with Zn 2+, In3+, and Ga3+/2+ to modify its catalytic properties, thanks the synergy of two cations and/or with the creation of vacancies in the structure.(5)

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